On the hyperbolicity of Grad's moment system in gas kinetic theory

Yuwei Fan

Department of Mathematics, Stanford University

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based on the work jointed with

- Zhenning Cai, Duke University, NC
- Ruo Li, Peking University, China

Outline

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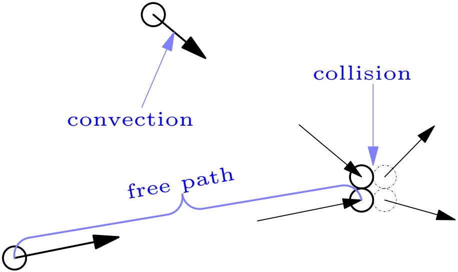
Gas kinetic theory



$$Kn = \frac{\text{Mean free path } \lambda}{\text{typical length scale } L}$$



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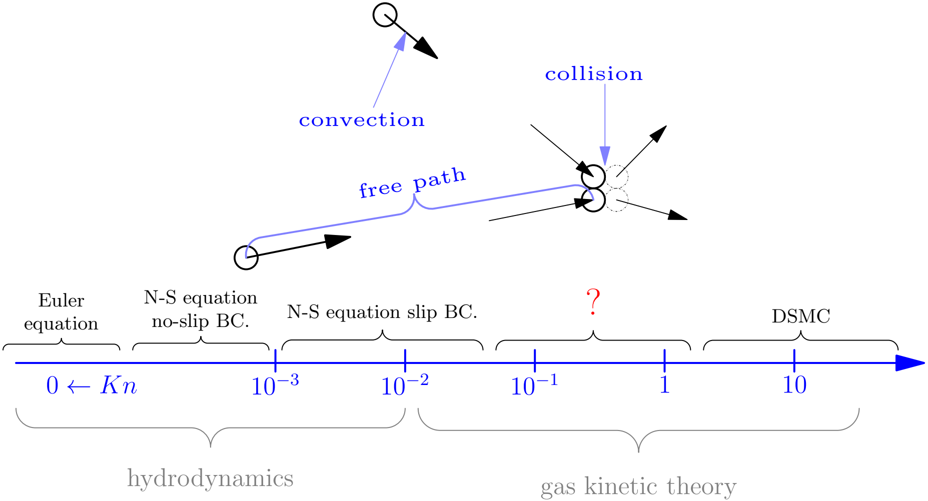

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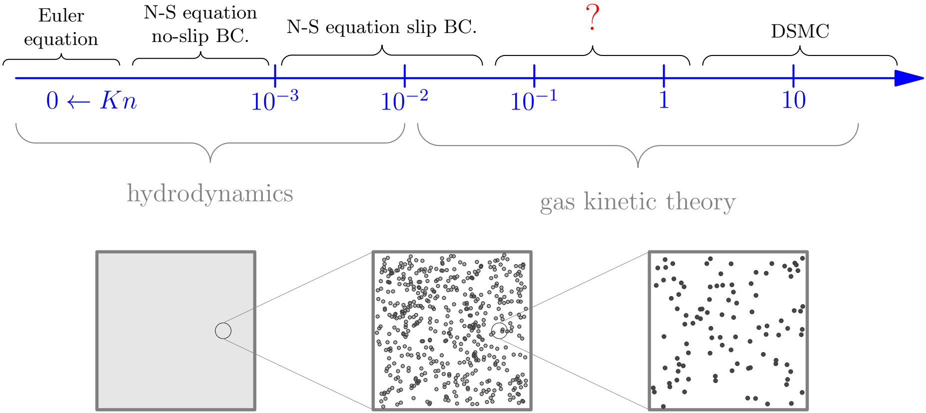
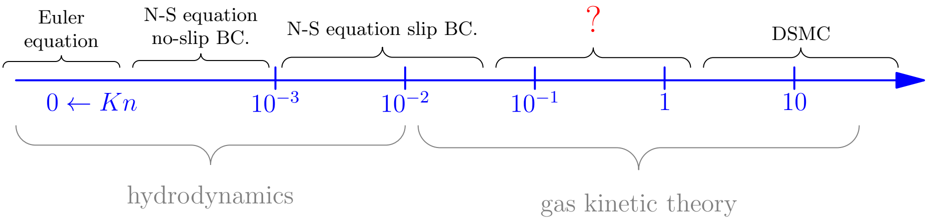
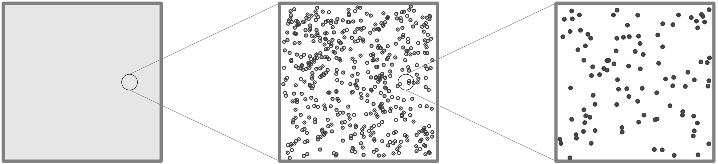


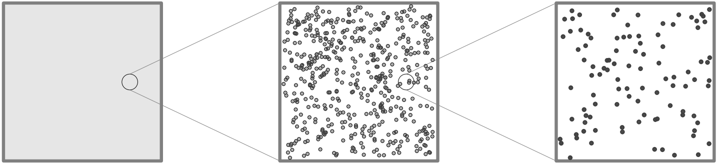
Gas kinetic theory





densy gas	→	rarefied gas	→	very rarefied gas
↓		↓		↓
hydrodynamics		?		molecular dynamics
↓		↓		↓
Continuum mechanics	→	?	←	molecular motion

Gas kinetic theory



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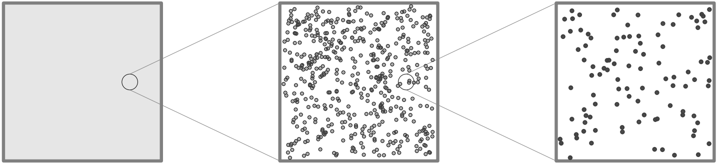
				$\delta(\boldsymbol{x}_i(t), \boldsymbol{p}_i(t))$

Gas kinetic theory



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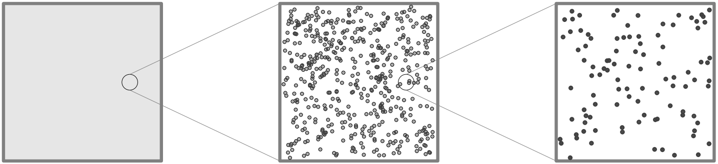
Continuum mechanics	$\rightarrow$	?	$\leftarrow$	molecular motion
$\downarrow$				$\downarrow$
		$f(t, \boldsymbol{x}, \boldsymbol{p}) = \sum_i \delta(\boldsymbol{x}_i, \boldsymbol{p}_i)$	$\leftarrow$	$\delta(\boldsymbol{x}_i(t), \boldsymbol{p}_i(t))$

Distribution function: $f(t, \boldsymbol{x}, \boldsymbol{\xi})$, $(\boldsymbol{\xi} = \boldsymbol{p}/m)$

Gas kinetic theory



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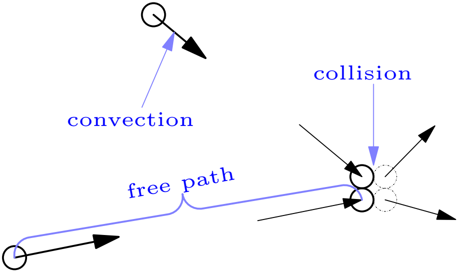
Continuum mechanics	→	?	←	molecular motion
↓		⇑		↓
$\int_{\mathbb{R}^3} (1, \boldsymbol{p}, \lvert\boldsymbol{p}\rvert^2) f \, \mathrm{d}\boldsymbol{p}$	←	$f(t, \boldsymbol{x}, \boldsymbol{p}) = \sum_i \delta(\boldsymbol{x}_i, \boldsymbol{p}_i)$	←	$\delta(\boldsymbol{x}_i(t), \boldsymbol{p}_i(t))$

Distribution function: $f(t, \boldsymbol{x}, \boldsymbol{\xi})$, $(\boldsymbol{\xi} = \boldsymbol{p}/m)$

Boltzmann Equation



Boltzmann equation (Boltzmann 1872) reads:

$$\frac{\partial f}{\partial t} + \underbrace{\boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f}_{\text{Convection}} = \underbrace{Q(f, f)}_{\text{Collision}},$$

$Q(f, f)$ is collision term, and $(t, \boldsymbol{x}, \boldsymbol{\xi}) \in \mathbb{R}^+ \times \mathbb{R}^D \times \mathbb{R}^D$.

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Notations:

$\rho \rightarrow$ density	$\boldsymbol{u} \rightarrow$ macroscopic velocity
$T \rightarrow$ tempurature	$\sigma_{ij} \rightarrow$ stress tensor
$\rho T_{ij} = \rho T \delta_{ij} + \sigma_{ij} \rightarrow$ press tensor	$q_i \rightarrow$ heat flux.

Local equilibrium : (Maxwell 1860)

$$\mathcal{M}(t, \boldsymbol{x}, \boldsymbol{\xi}) = \frac{\rho(t, \boldsymbol{x})}{\sqrt{2\pi T(t, \boldsymbol{x})}^D} \exp\left(-\frac{|\boldsymbol{\xi} - \boldsymbol{u}(t, \boldsymbol{x})|^2}{2T(t, \boldsymbol{x})} \right)$$

Difficulties in Solving Boltzmann Equation

Boltzmann equation (Boltzmann 1872) reads:

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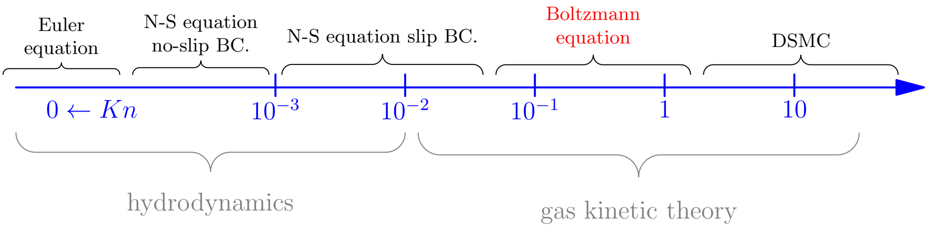
1. Complex collision term $Q(f, f)$, e.g. binary collision term:

$$Q(f, f) = \int_{\mathbb{R}^3} \int_{S^+} (f' f_1' - f f_1) B(|\boldsymbol{\xi} - \boldsymbol{\xi}_1|, \sigma) \, \mathrm{d}\boldsymbol{\xi}_1 \, \mathrm{d}\boldsymbol{n};$$

2. High-order variable: 1 (t) + D($\boldsymbol{x}$) + D($\boldsymbol{\xi}$) = 2D+1;
3. $\boldsymbol{\xi} \in \mathbb{R}^3$.

Start Point of Moment Method



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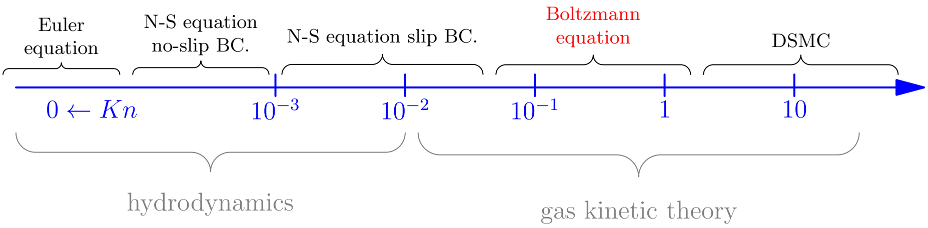
$\int_{\mathbb{R}^3}(1,\boldsymbol{\xi},\lvert\boldsymbol{\xi}\rvert^2)f\,\mathrm{d}\boldsymbol{\xi}$	$\leftarrow$	$f(t,\boldsymbol{x},\boldsymbol{\xi})=\sum_i \delta(\boldsymbol{x}_i,\boldsymbol{\xi}_i)$	$\leftarrow$	$\delta(\boldsymbol{x}_i(t),\boldsymbol{\xi}_i(t))$

Start Point of Moment Method



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Boltzmann equation $\Longrightarrow$ Hydrodynamic equations

$\uparrow$

Moment method

Moment method

$$\begin{array}{rcl} \mathbb{M} & \rightarrow & \text{finite-dimensional subspace of } D\text{-variate polynomials} \\ \{m_i(\boldsymbol{\xi})\}_{i=0}^{M} & \rightarrow & \text{a basis of } \mathbb{M}, \quad \boldsymbol{m} = (m_0, \cdots, m_M)^T \\ \mu_i = \langle f m_i \rangle & \rightarrow & \text{moments, concerned with in the issue} \\ \boldsymbol{\mu} & \rightarrow & (\mu_0, \dots, \mu_M)^T \end{array}$$

Moment equations:

$$\frac{\partial \mu_i}{\partial t} + \sum_{d=1}^{D} \frac{\partial \langle \xi_d m_i(\boldsymbol{\xi}) f \rangle}{\partial x_d} = \langle m_i Q(f,f) \rangle \qquad (1)$$

Moment closure: Give the state equations of $\langle \xi_d m_i(\boldsymbol{\xi}) f \rangle$ and $\langle m_i Q(f,f) \rangle$, $d = 1, \dots, D, i = 0, \dots, M$ by $\boldsymbol{\mu}$.

$$\frac{\partial \boldsymbol{\mu}}{\partial t} + \sum_{d=1}^{D} \frac{\partial \boldsymbol{F}_d(\boldsymbol{\mu})}{\partial x_d} = \boldsymbol{Q}(\boldsymbol{\mu})$$

Good Model or Bad Model

- Well-posedness of the model:

  Hyperbolicity, Stability,$\cdots$

- Preserving of physics:

  Conservation, H-theorem, Galilean invariance, $\cdots$

- Approximation efficiency:

  # DOF vs Accuracy

- Implementation:

  BC, Easy to implement,...

Hyperbolicity

Definition (Globally Hyperbolic)

The first-order equations

$$\frac{\partial \boldsymbol{w}}{\partial t} + \mathbf{A}(\boldsymbol{w})\frac{\partial \boldsymbol{w}}{\partial x} = 0$$

is globally hyperbolic if the coefficient matrix $\mathbf{A}(\boldsymbol{w})$ is diagonalizable with real eigenvalues for any admissible $\boldsymbol{w}$.

What if the system is not hyperbolic?

Hyperbolicity

Example

The initial value problem

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} 0 & a \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x}\begin{pmatrix} u \\ v \end{pmatrix} = 0, \quad \begin{pmatrix} u(x,0) \\ v(x,0) \end{pmatrix} = \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix}.$$

The characteristic speeds of the system is $\sqrt{a}$ and $-\sqrt{a}$, and the system is hyperbolic if and only if $a > 0$.

This system can be reduced as

$$\begin{cases} u_{tt} - a u_{xx} = 0, \\ u(x,0) = u_0(x), \\ u_t(x,0) = -a v_{0,t}(x). \end{cases}$$

If a is negative, for example $a = -1$, the system turns to be elliptic equation with two boundary conditions, resulting in the inexistence of weak solution of the system.

Outline

Grad's moment method(Grad 1949)

Idea: Assume f is not far from the local equilibrium $f_{\rm eq}$,

$$f \sim f_{\rm eq}.$$

Grad's expansion: expand the distribution around f_{eq}:

$$f = f_{\rm eq} \sum_{\alpha\in\mathbb{I}} g_\alpha He_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi}) = \sum_{\alpha\in\mathbb{I}} f_\alpha \mathcal{H}_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi}).$$

Moment closure: $$f_\alpha = \frac{T^{|\alpha|}}{\alpha!}\left\langle f He_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi})\right\rangle$$

Orthogonal polynomial: Hermite polynomial

$$He_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi}) = \frac{(-1)^{|\alpha|}}{\omega^{[\boldsymbol{u},T]}(\boldsymbol{\xi})}\frac{\partial^\alpha \omega^{[\boldsymbol{u},T]}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}^\alpha}, \quad \omega^{[\boldsymbol{u},T]}(\boldsymbol{\xi}) = \frac{f_{\rm eq}}{\rho},$$

Basis function:

$$\mathcal{H}_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi}) = \omega^{[\boldsymbol{u},T]}(\boldsymbol{\xi}) He_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi}).$$

Grad's moment method(Grad 1949)

Grad's expansion:

$$f(t,\boldsymbol{x},\boldsymbol{\xi}) = \sum_{\alpha\in\mathbb{I}} f_\alpha \mathcal{H}_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi}).$$

Properties of Grad's expansion:

- Constraints:

$$f_0 = \rho, \quad f_{e_d} = 0,\ d = 1,\cdots,D, \quad \sum_{d=1}^{D} f_{2e_d} = 0.$$

- First term is Maxwellian:

$$f_0\mathcal{H}_0^{[\boldsymbol{u},T]}(\boldsymbol{\xi}) = f_{\text{eq}}.$$

- Basis functions depend on t, $\boldsymbol{x}$.

$$\frac{\partial \mathcal{H}_\alpha^{[\boldsymbol{u},T]}(\boldsymbol{\xi})}{\partial s} = \sum_{i=1}^{D} \mathcal{H}_{\alpha+e_i}^{[\boldsymbol{u},T]}(\boldsymbol{\xi})\frac{\partial u_i}{\partial s} + \frac{1}{2}\frac{\partial T}{\partial s}\sum_{i=1}^{D}\mathcal{H}_{\alpha+2e_i}^{[\boldsymbol{u},T]}(\boldsymbol{\xi}), \quad s = t, x_d.$$

Grad's Moment Method

Grad's expansion: $f = \sum_{\boldsymbol{\alpha} \in \mathbb{I}} f_{\boldsymbol{\alpha}} \mathcal{H}_{\boldsymbol{\alpha}}^{[\boldsymbol{u},T]}(\boldsymbol{\xi})$

$\downarrow$ substitute into

Boltzmann Equation: $\frac{\partial f}{\partial t} + \boldsymbol{\xi} \nabla f = Q(f, f)$

$\downarrow$ matching coefficients(Galerkin)

Grad's Moment Equations: $\frac{\partial \boldsymbol{w}_M}{\partial t} + \sum_{d=1}^{D} \mathbf{A}_{d,M}(\boldsymbol{w}_M) \frac{\partial \boldsymbol{w}_M}{\partial x_d} = \boldsymbol{Q}_M$

Grad's 13 Moment System

Grad's 13 moment expansion [Grad 1949]:

$$f|_{G13} = f_{eq}\left[1 + \frac{T_{ij} - \delta_{ij}T}{2T^2}\left(C_iC_j - \delta_{ij}C^2\right) + \frac{2}{5}\frac{q_k}{\rho T^2}C_k\left(\frac{C^2}{2T} - \frac{5}{2}\right)\right],$$

where $C_i = \xi_i - u_i$ is the relative velocity.

$$\mathbb{M} = \{1, \boldsymbol{\xi}, \boldsymbol{\xi}\otimes\boldsymbol{\xi}, \boldsymbol{\xi}|\boldsymbol{\xi}|^2\}.$$

Substituting the expansion into the Boltzmann equation, and matching the coefficients of the polynomials, we can obtain the well-known Grad's 13 moment system

Grad's 13 Moment System

$$
\begin{aligned}
&\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \frac{\partial u_k}{\partial x_k} = 0, \\
&\frac{\mathrm{d}u_i}{\mathrm{d}t} + \frac{T_{ik}}{\rho}\frac{\partial \rho}{\partial x_k} + \frac{\partial T_{ik}}{\partial x_k} = 0, \\
&\frac{\mathrm{d}T_{ij}}{\mathrm{d}t} + 2T_{k(i}\frac{\partial u_{j)}}{\partial x_k} + \frac{1}{\rho}\left(\frac{4}{5}\frac{\partial q_{(i}}{\partial x_{j)}} + \frac{2}{5}\delta_{ij}\frac{\partial q_k}{\partial x_k}\right) = Q(T_{ij}), \\
&\frac{\mathrm{d}q_i}{\mathrm{d}t} - (T_{ij}T_{jk} - 2TT_{ik} + T^2\delta_{ik})\frac{\partial \rho}{\partial x_k} + \frac{7}{5}q_i\frac{\partial u_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial u_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial u_k}{\partial x_i} \\
&\qquad - \rho T_{ik}\left(\frac{\partial T_{jk}}{\partial x_j} - \frac{7}{6}\frac{\partial T_{jj}}{\partial x_k}\right) + 2\rho T\left(\frac{\partial T_{ik}}{\partial x_k} - \frac{1}{3}\frac{\partial T_{jj}}{\partial x_i}\right) = Q(q_i).
\end{aligned}
$$

Outline

Hyperbolicity of Grad's 13 Moment System: 1D case

1D case: Grad's 13 moment system degenerates into

$$\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}t} + \mathbf{A}(\boldsymbol{w})\frac{\partial \boldsymbol{w}}{\partial x} = Q(\boldsymbol{w}) \tag{2}$$

where $\boldsymbol{w} = (\rho, u_1, T_{11}, T_{22}, q_1)^T$,

$$\mathbf{A}(\boldsymbol{w}) = \begin{pmatrix} 0 & \rho & 0 & 0 & 0 \\ T_{11}/\rho & 0 & 1 & 0 & 0 \\ 0 & 2T_{11} & 0 & 0 & \frac{6}{5\rho} \\ 0 & 0 & 0 & 0 & \frac{2}{5\rho} \\ -4(T_{11}-T_{22})^2/9 & 16q_1/5 & \rho(11T_{11}+16T_{22})/18 & \rho(17T_{11}-8T_{22})/9 & 0 \end{pmatrix}.$$

The characteristic polynomial is

$$\det(\lambda\mathbf{I} - \mathbf{A}) = \lambda\left[\lambda^4 - \frac{2}{45}(101T_{11} + 16T_{22})\lambda^2 - \frac{96}{25}\frac{q_1}{\rho}\lambda + \frac{1}{15}(53T_{11}^2 - 16T_{11}T_{22} + 8T_{22}^2)\right],$$

which only depends on $\frac{\sigma_{11}}{\rho}$ and $\frac{q_1}{\rho}$. ($T_{11} = T + \sigma_{11}/\rho, T_{22} = T - \sigma_{11}/2\rho$)

Hyperbolicity of Grad's 13 Moment System: 1D case

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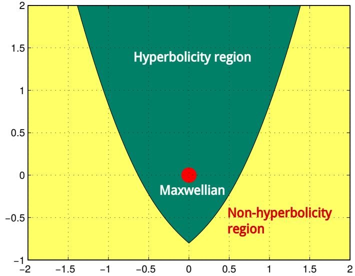

Figure 1: x-axis: $\frac{q_1}{\rho T^{3/2}}$, y-axis: $\frac{\sigma_{11}}{\rho T}$

Hyperbolicity of Grad's 13 Moment System: 1D case

1D case: Grad's 13 moment system degenerates into

$$\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}t} + \mathbf{A}(\boldsymbol{w})\frac{\partial \boldsymbol{w}}{\partial x} = Q(\boldsymbol{w}) \tag{2}$$

Result:

- (2) is not globally hyperbolic (I. Muller 1998)
- Maxwellian is an inner point of hyperbolicity region

Hyperbolicity of Grad's 13 Moment System: 3D case

3D case: Write Grad's 13 Moment System in quasi-linear form:

$$\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}t} + \sum_{d=1}^{3} \mathbf{A}_d \frac{\partial \boldsymbol{w}}{\partial x_d} = Q(\boldsymbol{w}),$$

where

$$\boldsymbol{w} = (\rho, u_1, u_2, u_3, T_{11}, T_{22}, T_{33}, T_{12}, T_{13}, T_{23}, q_1, q_2, q_3)^T.$$

It is enough to examine $\mathbf{A}_1$ due to the rotational invariance.

Hyperbolicity of Grad's 13 Moment System: 3D case

For the Gaussian distribution

$$f = \frac{\rho}{\sqrt{\det(2\pi\boldsymbol{\Theta})}} \exp\left(-\frac{1}{2}\boldsymbol{C}^T\boldsymbol{\Theta}^{-1}\boldsymbol{C}\right), \ \boldsymbol{\Theta} = \begin{pmatrix} T & \epsilon T & 0 \\ \epsilon T & T & 0 \\ 0 & 0 & T \end{pmatrix},$$

where $|\epsilon| < 1$, the characteristic polynomial of $\mathbf{A}_1$ is

$$\det(\lambda\mathbf{I} - \mathbf{A}_1) = \frac{(\lambda - u_1)^3}{125}[5(\lambda - u_1)^2 - 7T] \cdot g\left(\frac{(\lambda - u_1)^2}{T}\right),$$

$$g(x) = 25x^4 - 165x^3 + \left(257 + 48\epsilon^2\right)x^2 + \left(8\epsilon^2 - 105\right)x - 28\epsilon^2.$$

$g(x)$ has at least one negative zero

⇓

$\mathbf{A}_1$ has at least two complex eigenvalues

⇓

Grad 13 is NOT hyperbolic near **Maxwellian**

Hyperbolicity of Grad's 13 Moment System: 3D case

Hyperbolicity region of Grad 13 moment system on the $T_{12} - q_1$ plane is:

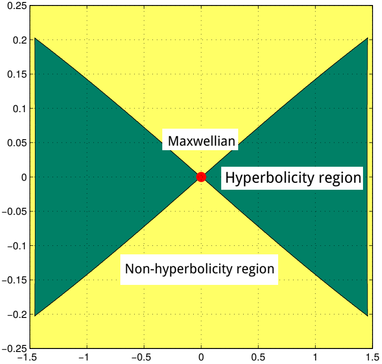

Figure 1: x-axis: $\frac{q_1}{\rho T^{3/2}}$, y-axis: $\frac{T_{12}}{T}$

Hyperbolicity of Grad's 13 Moment System

1D case:

- The system is not globally hyperbolic (I. Muller 1998)
- Maxwellian is an inner point of hyperbolicity region

3D case: (Cai, Fan and Li, KRM 2014)

- Grad's 13 moment system is not globally hyperbolic
- Maxwellian is NOT an inner point of hyperbolicity region

Hyperbolicity of Grad's 13 Moment System

1D case:

- The system is not globally hyperbolic (I. Muller 1998)
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3D case: (Cai, Fan and Li, KRM 2014)

- Grad's 13 moment system is not globally hyperbolic
- Maxwellian is NOT an inner point of hyperbolicity region

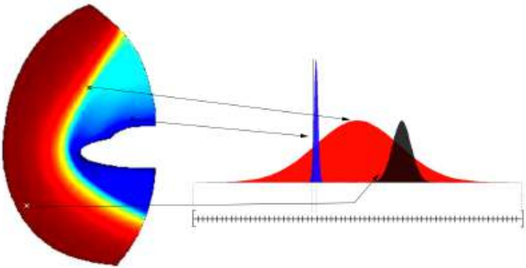
Question:

1. Why we care about the hyperbolicity?
2. Why Grad's moment systems is not globally hyperbolic?
3. How to fix the loss of hyperbolicity of Grad's moment system?

Example: Adaptive discrete velocity method

Discrete velocity method for BGK: discrete points $\xi_k = k\Delta v$, $\Delta v = L/N$, $k = -N, \ldots, N$, $f_k = f(\xi_k)$,

$$\frac{\partial f_k}{\partial t} + \xi_k \frac{\partial f_k}{\partial x} = \frac{1}{\tau}(f_k^{eq} - f_k)$$



Constraints on the velocity grid(S. Brull et.al 2014)

- Large enough bounds

$$L \geq \max_{t,x}(u(t,x) + c\sqrt{T(t,x)}), \quad -L \leq \min_{t,x}(u(t,x) - c\sqrt{T(t,x)})$$

- small enough grid step

$$\Delta v \leq \min_{t,x} \sqrt{T(t,x)}$$

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Adaptive discrete velocity(S. Brull et.al 2014) discrete points: $\xi_k = u(t,x) + k\Delta v\sqrt{T(t,x)}$
Transformation:

$$\tilde{f}(t,x,v) = \frac{\sqrt{T(t,x)}}{\rho(t,x)} f(t,x,u(t,x) + \sqrt{T(t,x)}v)$$

Governing equation: (equivalent to solve the following equation by DVM)

$$\begin{aligned}&\left(\frac{\mathrm{dln}(\rho)}{\mathrm{d}t} - \frac{3}{2}\frac{\mathrm{dln}(T)}{\mathrm{d}t}\right)\tilde{f} + \frac{\mathrm{d}\tilde{f}}{\mathrm{d}t} - \sum_{j=1}^{3}\frac{\partial \tilde{f}}{\partial v_j}\left(\frac{1}{\sqrt{T}}\frac{\mathrm{d}u_j}{\mathrm{d}t} + \frac{v_j}{2}\frac{\mathrm{dln}(T)}{\mathrm{d}t}\right)\\
&+\sum_{d=1}^{3}\sqrt{T}v_d\left(\left(\frac{\partial \ln(\rho)}{\partial x_d} - \frac{3}{2}\frac{\partial \ln(T)}{\partial x_d}\right)\tilde{f} + \frac{\partial \tilde{f}}{\partial x_d} - \sum_{j=1}^{3}\frac{\partial \tilde{f}}{\partial v_j}\left(\frac{1}{\sqrt{T}}\frac{\partial u_j}{\partial x_d} + \frac{v_j}{2}\frac{\partial \ln(T)}{\partial x_d}\right)\right)\\
&= \frac{1}{\tau}(\tilde{f}_{eq} - \tilde{f})\end{aligned}$$

Recent development

- Regularized moment method: parabolic equations, not first-order equations
  R13(H. Struchtrup, M. Torrilhon 2003)
  R26(X. Gu et. al 2009)
  NRxx(Z. Cai, R. Li 2012)
- Hyperbolic regularized moment method: globally hyperbolic
  Globally hyperbolic moment system (Z. Cai, Y. Fan, R. Li, 2013, 2014)
  Generalized framework for kinetic equation(Z. Cai, Y. Fan, R. Li, 2015; Y. Fan et. al 2016)
- Approximate moment method: properties V.S implement
  Approximate 14 moment system (J. McDonald and M. Torrilhon, 2013)
  Bi-Gaussian based moment system (in preparation)

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Thank you for your attention!